

## Derivation of a Numerical Method for solving a single nonlinear parabolic PDE

### I. FORMULATION.

Nonlinear parabolic partial differential equations are, in their most general form, given by:

$$\frac{\partial T}{\partial t} = K(x, t, T, \nabla T, \nabla^2 T) \quad (I.1)$$

An example of this is the general form of the linear parabolic PDE, which we solved in the last section.

$$\frac{\partial T}{\partial t} = \nabla \cdot [c(\nabla T)] - aT - \underline{b} \cdot \nabla T + f \quad (I.2)$$

Another example is

$$\frac{\partial T}{\partial t} = \nabla \cdot [c(\nabla T)] - aT^2 - \underline{b} \cdot \nabla T + f \quad (I.3)$$

Because equation (I.3) is no longer linear in the temperature and its derivatives, the techniques for solving linear parabolic PDEs, e.g. the Crank-Nicolson method no longer apply. We cannot reduce equation (I.3) to a discrete system of linear equations.

We proceed to solve the general nonlinear parabolic partial differential equation by discretizing space and time, as was done for the linear case. We look at the one-dimensional case and divide our space dimension into  $m$  spatial increments, each of width  $\frac{L}{m}$ . If we are interested in observing the behavior from time  $t_o$  to  $t_f$ , then we can divide that time into  $n$  equal temporal increments, each of width  $\frac{t_f - t_o}{n}$ . See Figure One, last section. We know our initial conditions and boundary conditions as before. We require a formulation which will allow us to incrementally solve the P.D.E through time. Where we could then obtain  $T(t_1, \{x\})$  from  $T(t_o, \{x\})$  and  $T(t, x_o)$  and  $T(t, x_m)$ . In general we want to obtain  $T(t_{j+1}, \{x\})$  from  $T(t_j, \{x\})$  and  $T(t, x_o)$  and  $T(t, x_m)$ .

We will derive one such method, based on the second-order Runge-Kutta method.

## II. DISCRETIZATION.

Derivation of the Runge-Kutta finite difference equations for nonlinear parabolic PDEs

### A. The Parabolic partial differential equation.

Let  $j$  superscripts designate temporal increments and let  $i$  subscripts designate spatial increments. For purposes of brevity only, we will consider the case with variation only in one spatial dimension. The extension to three dimensions is straightforward. Our most general parabolic PDE becomes in one spatial dimension

$$\frac{\partial T}{\partial t} = K(x, t, T, \nabla T, \nabla^2 T) \quad (\text{I.1})$$

Looking at it in this light, we can obtain a new estimate of the temperature, one increment ahead in time, namely

$$\left( \frac{\partial T}{\partial t} \right)_i \approx \frac{T_i^{j+1} - T_i^j}{t_{j+1} - t_j} = \frac{T_i^{j+1} - T_i^j}{\Delta t} \quad (\text{II.1})$$

This statement is true at any given point  $i$  in space. It is a can make a forward finite difference formula of the partial derivative with respect to time. Now what is also true by the second-order Runge-Kutta method is that:

$$\begin{aligned} \left( \frac{\partial T}{\partial t} \right)_i &\approx \frac{1}{2} \left[ K(x_i, t_{j+1}, T^{j+1}, \nabla T^{j+1}, \nabla^2 T^{j+1}) + K(x_i, t_j, T^j, \nabla T^j, \nabla^2 T^j) \right] \\ &= \frac{1}{2} \left[ K_i^{j+1} + K_i^j \right] \end{aligned} \quad (\text{II.2})$$

so that:

$$T_i^{j+1} = T_i^j + \frac{\Delta t}{2} \left[ K_i^{j+1} + K_i^j \right] \quad (\text{II.3})$$

The problem here is that we have no way of determining  $T_i^{j+1}$ , which is used as an argument in  $K_i^{j+1}$  unless we rely on a costly and inefficient method for finding the roots of a system of non-linear algebraic equations at each time iteration. This method is, of course, an option, but if we only want second order accuracy in our model, there are other, easier ways to get it.

The second-order Runge-Kutta method actually says that we should evaluate the function  $K_i^{j+1}$  as  $K(x_i, t_{j+1}, T_i^j + \Delta t K_i^j)$ . Since  $K_i^j$  is the time derivative of  $T_i^j$ , an estimate of the temperature  $T_i^{j+1}$  is

$$T_i^{j+1} \approx T_i^j + \Delta t K_i^j \quad (\text{II.4})$$

so that

$$T_i^{j+1} = T_i^j + \frac{\Delta t}{2} \left[ K_i^{j+1} + K_i^j \right] \quad (\text{II.5})$$

This is the formula for the second-order Runge-Kutta, when applied to ODEs. This is also known as Heun's method with one iteration.

It is important to see that these  $K_i^j$  are functions not only of  $T_i^j$  but of the temperature at all spatial points  $\{ T^j \}$ . So we have to solve a system of ODEs simultaneously. Easy stuff for the Runge-Kutta method.

Also, we need to recognize that the gradients and laplacians inside  $K_i^j$  must be evaluated using the same finite difference formulae as were used in the linear case, namely:

$$\left( \frac{\partial T}{\partial x} \right)_i^j \approx \frac{T_{i+1}^j - T_{i-1}^j}{x_{i+1} - x_{i-1}} = \frac{T_{i+1}^j - T_{i-1}^j}{2\Delta x} \quad (\text{II.6})$$

and

$$\left( \frac{\partial^2 T}{\partial x^2} \right)_i^j \approx \frac{\left( \frac{T_{i+1}^j - T_i^j}{\Delta x} \right) - \left( \frac{T_i^j - T_{i-1}^j}{\Delta x} \right)}{\Delta x} = \frac{T_{i+1}^j - 2T_i^j + T_{i-1}^j}{\Delta x^2} \quad (\text{II.7})$$

The algorithm then is as follows:

1. at time  $j=0$ , obtain  $T_i^j$  for all  $i$  from initial conditions.
2. using (II.6) and (II.7), calculate first and second spatial partial derivatives for all  $i$  at time  $j$ .
3. calculate  $K_i^j$  for all  $i$

4. calculate new estimate of  $T_i^{j+1}$  from equation (II.4)
5. using (II.6) and (II.7), calculate first and second spatial partial derivatives for all  $i$  at time  $j+1$ .
6. calculate  $K_i^{j+1}$  for all  $i$
7. calculate new value of  $T_i^{j+1}$  from equation (II.5)
8.  $j = j+1$  and loop back to step 2 for next temporal iteration

*B. Initial Conditions.*

The initial conditions should give  $T_i^{j=0}$ , so that they can be used in the same way that initial conditions to an ODE problem using Runge-Kutta are used.

*C. Boundary Conditions.*

1. Dirichlet

Dirichlet boundary conditions give the value of the temperature at the boundaries. This means that the boundary nodes are known at all times and do not need to be integrated using Runge-Kutta. If there are  $m$  spatial intervals, then there are  $m+1$  spatial nodes, but only  $m-1$  of those spatial nodes will be integrated through time.

2. Neumann

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